PHYSICAL REVIEW E VOLUME 52, NUMBER 5 NOVEMBER 1995

Variational path-integral approach to a nonlinear open system

Jing-Dong Bao,[1,*] Yi-Zhong Zhuo,[2] and Xi-Zhen Wu[2]
[1]Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100080, China
[2]Institute of Atomic Energy, P.O. Box 275, Beijing 102413, China
(Received 12 September 1994; revised manuscript received 30 May 1995)

The variational path-integral method is used to calculate the partition function with an effective potential of a nonlinear open system, which is described by the system-plus-environment model. The two variational parameters corresponding to the potential and the coupling form factor, respectively, in the quadratic trial action are determined by minimizing the effective potential. A general expression for the partition function at finite temperature is obtained.

PACS number(s): 05.30.−d, 03.65.Db, 02.50.−r

I. INTRODUCTION

The variational approach to path integrals was developed first by Feynman as early as 1972 [1]. In the last decade, a considerable improvement on Feynman's original variational approximation has been put forward by Giachetti and Tognetti [2], and independently by Feynman and Kleinert [3]. The basic idea of the refined treatment is to make up a quadratic trial action and to use the affiliated frequency as a variational parameter; the result leads a second-order effective potential. This method can yield realistic thermodynamic properties of quantum statistical systems and it also requires much less computer time. Then the variational path-integral theory has been applied successfully to several nonlinear statistical systems [4–7]; some comparative studies of a model using the quantum Monte Carlo and effective potential methods were also done in [8]. Only very recently, Kleinert and co-workers [9] proposed corrections of this method for the anharmonic potential carried out to higher-order terms. However, the theory so far has been limited to conservative systems and the case of linear coupling between the collective coordinate and the environmental oscillators [10]. In the present paper we apply the variational path-integral formulation to calculate the effective potential of a nonlinear quantum open (dissipative) system.

II. MODEL AND FORMULAS

The system under study is governed by the Lagrangian

$$L=\tfrac{1}{2}m\dot{x}^2-V(x)+\sum_{\alpha=1}^{\infty}\frac{m_\alpha}{2}\left\{\dot{q}_\alpha^2-\omega_\alpha^2\left[q_\alpha-\frac{c_\alpha}{m_\alpha\omega_\alpha}f(x)\right]^2\right\}, \quad (1)$$

where x and q_α are the collective coordinate and the coordinates of the environmental oscillators, respectively, and the coupling form factor $f(x)$ is assumed to be a general function of the collective coordinate. Note that here the coupling term is written in a form that does not induce a renormalization of the potential [11,12].

We start with the Feynman path-integral form of the partition function. By eliminating the environmental degrees of freedom [1], the partition function at temperature $k_BT=1/\beta$ can be expressed only by an integral over the collective coordinate $x(\tau)$ as

$$Z(\beta)=\int D[x]\exp[-S_{\rm eff}(x)/\hbar] \ . \quad (2)$$

Here the effective action $S_{\rm eff}(x)$ is given by

$$S_{\rm eff}(x)=\int_0^{\hbar\beta}[\tfrac{1}{2}m\dot{x}^2+V(x)]d\tau+\tfrac{1}{2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau' k(\tau-\tau')\times f(x(\tau))f(x(\tau')), \quad (3)$$

where the last term describes the influence of the environment. In Eq. (3), the influence kernel $k(\tau)$ is given by

$$k(\tau-\tau')=\sum_{\alpha=1}^{\infty}\left\{\frac{c_\alpha^2}{m_\alpha\omega_\alpha^2}:\delta(\tau-\tau'):-\frac{c_\alpha^2}{2m_\alpha\omega_\alpha}\frac{\cosh[\omega_\alpha(|\tau-\tau'|-0.5\hbar\beta)]}{\sinh(0.5\hbar\beta\omega_\alpha)}\right\}, \quad (4)$$

where $:\delta(\tau-\tau'):$ is a generalized delta function with a period $\hbar\beta$.

The paths are periodic and may be represented as a Fourier series

$$x(\tau)=x_0+x_1(\tau)=x_0+\sum_{n=1}^{\infty}[x_n\exp(i\theta_n\tau)+\text{ c.c.}] \ , \quad (5)$$

where $\theta_n=2\pi n/\hbar\beta$ are the Matsubara frequencies, $x_0=(1/\hbar\beta)\int_0^{\hbar\beta}x(\tau)d\tau$ is the average path, and $x_n=x_n^{\rm Re}+ix_n^{\rm Im}=x_{-n}^*$.

Using a measure of the product of integrals of all Fourier components [10], the partition function then has the appearance of a classical partition function with an effective potential $W(x_0)$:

$$Z=\int_{-\infty}^{\infty}\left[\frac{m}{2\pi\hbar^2\beta}\right]^{1/2}dx_0\exp[-\beta W(x_0)] \ . \quad (6)$$

The effective potential can be written

*Mailing address: Beijing Institute of Meteorology, Beijing 100081, China.

$$\exp[-\beta W(x_0)]=\int D[x_1]\exp\left\{-m\beta\sum_{n=1}^{\infty}\theta_n^2|x_n|^2-\frac{1}{\hbar}\int_0^{\hbar\beta}V(x_0+x_1(\tau))d\tau\right.$$
$$\left.-\frac{1}{2\hbar}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau' k(\tau-\tau')f(x_0+x_1(\tau))f(x_0+x_1(\tau'))\right\}. \tag{7}$$

To find a simple but very accurate approximation to $W(x_0)$, we make up a quadratic trial action. The main idea is to decompose the potential as well as the coupling form factor into

$$V(x(\tau))=\tfrac{1}{2}m\Omega^2(x_0)[x(\tau)-x_0]^2+\tilde{V}(x(\tau)) \tag{8}$$

and

$$f(x(\tau))=\mu(x_0)[x(\tau)-x_0]+\tilde{f}(x(\tau)), \tag{9}$$

which involve the unknown x_0-dependent frequency function $\Omega^2(x_0)$ and slope function $\mu(x_0)$, which can be determined further by the variational method. This is an improvement over the Giachetti-Tognetti and Feynman-Kleinert original approach.

Substituting Eqs. (8) and (9) into (7), and representing the influence kernel $k(\tau)$ as a Fourier series

$$k(\tau)=\frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}K(\theta_n)\exp(i\theta_n\tau), \tag{10}$$

we perform the integral of the quadratic part of the effective action over the fluctuation modes,

$$Z_1(x_0)=\int D[x_1]\exp\left\{-m\beta\sum_{n=1}^{\infty}\left[\theta_n^2+\Omega^2(x_0)+\mu^2(x_0)\frac{K(\theta_n)}{m}\right]|x_n|^2\right\}$$
$$=\prod_{n=1}^{\infty}\theta_n^2\left[\theta_n^2+\Omega^2(x_0)+\mu^2(x_0)\frac{K(\theta_n)}{m}\right]^{-1}, \tag{11}$$

where $K(\theta_n)$ is the Laplace transform of $k(\tau)$ and is given by

$$K(\theta_n)=\sum_{\alpha=1}^{\infty}\frac{c_\alpha^2}{m_\alpha\omega_\alpha^2}\frac{\theta_n^2}{\omega_\alpha^2+\theta_n^2}. \tag{12}$$

Then Eq. (7) becomes

$$\exp[-\beta W(x_0)]=Z_1(x_0)\left\langle\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}\tilde{V}(x_0+x_1(\tau))d\tau\right.\right.$$
$$\left.\left.-\frac{1}{2\hbar}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau' k(\tau-\tau')\tilde{f}(x_0+x_1(\tau))\tilde{f}(x_0+x_1(\tau'))\right\}\right\rangle_1, \tag{13}$$

where $\tilde{V}(x(\tau))$ and $\tilde{f}(x(\tau))$ are determined by Eqs. (8) and (9), respectively, and the bracket $\langle\ \rangle_1$ denotes the expectation value calculated by the Gaussian probability distribution:

$$Z_1^{-1}(x_0)\exp\left\{-m\beta\sum_{n=1}^{\infty}\left[\theta_n^2+\Omega^2(x_0)+\mu^2(x_0)\frac{K(\theta_n)}{m}\right]|x_n|^2\right\}. \tag{14}$$

According to the Jensen-Peierls inequality, we have

$$Z_1(x_0)\left\langle\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\left[\tilde{V}(x(\tau))+\tfrac{1}{2}\tilde{f}(x(\tau))\int_0^{\hbar\beta}d\tau' k(\tau-\tau')\tilde{f}(x(\tau'))\right]\right\}\right\rangle_1$$
$$\geq Z_1(x_0)\exp\left\{-\beta\langle\tilde{V}(x(\tau))\rangle_1-\frac{1}{2\hbar}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau' k(\tau-\tau')\langle\tilde{f}(x(\tau))\tilde{f}(x(\tau'))\rangle_1\right\}, \tag{15}$$

in which $\langle\tilde{V}(x(\tau))\rangle_1$ arises from the original potential by smearing it out in the neighborhood of each point x_0 with the distribution (14) [3],

$$\langle\tilde{V}(x(\tau))\rangle_1=\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi a^2}}\tilde{V}(x)\exp\left[-\frac{(x-x_0)^2}{2a^2}\right]=\tilde{V}_{a^2}(x_0), \tag{16}$$

where

$$a^2(x_0)=\frac{2}{m\beta}\sum_{n=1}^{\infty}\left[\theta_n^2+\Omega^2(x_0)+\mu^2(x_0)\frac{K(\theta_n)}{m}\right]^{-1}. \tag{17}$$

On the right-hand side of Eq. (13) we still need to calculate the correlation function of the coupling form factor within the measure of the partition function $Z_1(x_0)$. For this we transform $\tilde{f}(x(\tau))$ into its Fourier components

$$\tilde{f}(x(\tau))=\int_{-\infty}^{\infty}\frac{dk}{2\pi}\exp[ikx(\tau)]\tilde{f}^*(k)\ . \tag{18}$$

Using the partition function $Z_1(x_0)$ in the form of (14), the expectation value now can be written as follows:

$$\begin{aligned}\langle\tilde{f}(x(\tau))\tilde{f}(x(\tau'))\rangle_1=Z_1^{-1}(x_0)\int D[x_1]\ \exp&\left\{-m\beta\sum_{n=1}^{\infty}\left[\theta_n^2+\Omega^2(x_0)+\mu^2(x_0)\frac{K(\theta_n)}{m}\right]|x_n|^2\right\}\\ &\times\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\tilde{f}^*(k_1)\tilde{f}^*(k_2)\\ &\times\exp\left\{ik_1\left[x_0+\sum_{n=1}^{\infty}[x_n\exp(i\theta_n\tau)+\text{c.c.}\right]\right\}\\ &\times\exp\left\{ik_2\left[x_0+\sum_{l=1}^{\infty}[x_l\ \exp(i\theta_l\tau')+\ \text{c.c.}]\right]\right\}\ .\end{aligned} \tag{19}$$

As far as the integrals over x_n are concerned in Eq. (19), those terms originating from the Fourier transform can be combined with the quadratic terms. Performing the integrals over x_n based on the verticality of the triangle function, we have

$$\langle\tilde{f}(x(\tau))\tilde{f}(x(\tau'))\rangle_1=\int\int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\tilde{f}^*(k_1)\tilde{f}^*(k_2)\ \exp[i(k_1+k_2)x_0-\tfrac{1}{2}a^2(x_0)(k_1^2+k_2^2)-b^2(x_0,\tau-\tau')k_1k_2]\ , \tag{20}$$

where $b^2(x_0,\tau-\tau')$ is the sum

$$b^2(x_0,\tau-\tau')=\frac{2}{m\beta}\sum_{n=1}^{\infty}\cos[\theta_n(\tau-\tau')]\left[\theta_n^2+\Omega^2(x_0)+\mu^2(x_0)\frac{K(\theta_n)}{m}\right]^{-1}\ . \tag{21}$$

Comparing (17) with (21), it is found that $b^2(x_0,\tau-\tau')\le a^2(x_0)$. It is also noticed that the time dependence in $x(\tau)$ has disappeared now. Inserting the Fourier representation of $\tilde{f}^*(k)$,

$$\tilde{f}^*(k)=\int_{-\infty}^{\infty}dx\ \tilde{f}(x)\ \exp(-ikx)\ , \tag{22}$$

we can perform the integral over k again via quadratic completion. Thus Eq. (20) becomes

$$\begin{aligned}\langle\tilde{f}(x(\tau))\tilde{f}(x(\tau'))\rangle_1=&\frac{1}{2\pi}(a^4-b^4)^{-1/2}\\ &\times\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dx_1dx_2\tilde{f}(x_1)\tilde{f}(x_2)\ \exp\left[-\frac{(x_1+x_2-2x_0)^2}{4(a^2+b^2)}-\frac{(x_1-x_2)^2}{4(a^2-b^2)}\right]\ .\end{aligned} \tag{23}$$

It is also quite easy to calculate the correlation function of the collective coordinate as

$$\langle x(\tau)x(\tau')\rangle_1=x_0^2+b^2(x_0,\tau-\tau'). \tag{24}$$

This is the desired result for the effective potential:

$$\begin{aligned}W_1(x_0)=&\frac{1}{\beta}\sum_{n=1}^{\infty}\ln\left[1+\frac{\Omega^2(x_0)}{\theta_n^2}+\mu^2(x_0)\frac{K(\theta_n)}{m\theta_n^2}\right]+V_{a^2}(x_0)-\tfrac{1}{2}m\Omega^2(x_0)a^2(x_0)\\ &+\frac{1}{2\hbar\beta}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau' k(\tau-\tau')\langle f(x(\tau))f(x(\tau'))\rangle_1\\ &-\frac{1}{\beta}\sum_{n=1}^{\infty}\mu^2(x_0)\frac{K(\theta_n)}{m}\left[\theta_n^2+\Omega^2(x_0)+\mu^2(x_0)\frac{K(\theta_n)}{m}\right]^{-1}\ .\end{aligned} \tag{25}$$

We are in a position to determine the two unknown trial functions $\Omega^2(x_0)$ and $\mu^2(x_0)$ by minimizing $W_1(x_0)$.

$$\begin{aligned}(W_1')_{\Omega^2}&=\frac{\partial W_1}{\partial\Omega^2}+\frac{\partial W_1}{\partial a^2}\frac{\partial a^2}{\partial\Omega^2}+\frac{\partial W_1}{\partial b^2}\frac{\partial b^2}{\partial\Omega^2}=0\ ,\\ (W_1')_{\mu^2}&=\frac{\partial W_1}{\partial\mu^2}+\frac{\partial W_1}{\partial a^2}\frac{\partial a^2}{\partial\mu^2}+\frac{\partial W_1}{\partial b^2}\frac{\partial b^2}{\partial\mu^2}=0\ .\end{aligned} \tag{26}$$

The results are

$$\Omega^2(x_0)=\frac{2}{m}\left[\frac{\partial V_{a^2}}{\partial a^2}+\delta\right]\ , \tag{27}$$

in which

$$\delta=\frac{1}{2\Delta}\sum_{l,n=1}^{\infty}\frac{[K^2(\theta_l)-K(\theta_l)K(\theta_n)]I_n}{A_l^2A_n^2} \tag{28}$$

and

$$\mu^2(x_0)=\frac{1}{\Delta}\sum_{l,n=1}^{\infty}\frac{[K(\theta_l)-K(\theta_n)]I_l}{A_l^2A_n^2}\ . \tag{29}$$

Here

$$\Delta=\sum_{l,n=1}^{\infty}\frac{K^2(\theta_l)-K(\theta_l)K(\theta_n)}{A_l^2A_n^2} \tag{30}$$

and

$$A_i=\theta_i^2+\Omega^2(x_0)+\mu^2(x_0)\frac{K(\theta_i)}{m} \quad (i=l,n,j) , \tag{31}$$

$$I_n=\frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau' k(\tau-\tau')\left[\frac{\partial}{\partial a^2}\langle f(x(\tau))f(x(\tau'))\rangle_1+\cos[\theta_n(\tau-\tau')]\frac{\partial}{\partial b^2}\langle f(x(\tau))f(x(\tau'))\rangle_1\right] . \tag{32}$$

The self-consistent equations (17), (21), and (27)–(31) must be solved numerically at each x_0, by iteration. Thus one can obtain the best upper bound $W_1(x_0)$ for the effective potential $W(x_0)$.

III. APPLICATION AND SUMMARY

In particular, when the dissipation between system and bath is linear, i.e., $f(x)=x$, we set

$$I_n=K(\theta_n), \quad I_l=K(\theta_l) , \tag{33}$$

then

$$\delta=0, \quad \mu^2=1 . \tag{34}$$

This is in agreement with [10].

As a simple physical application, we now consider a smooth coupling function $f(x(\tau))$ as a function of the fluctuation paths and expand it to second order near each average path x_0. This treatment is also applicable to many cases. With

$$f(x(\tau))\approx f(x_0)+f'(x_0)[x(\tau)-x_0] + \tfrac{1}{2}f''(x_0)[x(\tau)-x_0]^2 , \tag{35}$$

we find

$$\langle f(x(\tau))f(x(\tau'))\rangle_1 =f^2(x_0)+f(x_0)f''(x_0)a^2+f'^2(x_0)b^2 + \tfrac{1}{4}f''^2(x_0)(a^4+2b^4) . \tag{36}$$

Therefore

$$I_n=f'^2(x_0)K(\theta_n)+f''^2(x_0)\frac{1}{m\beta}\sum_{j=1}^{\infty}\frac{K(\theta_{j+n})}{A_j} . \tag{37}$$

Then

$$\delta(x_0)=\frac{f''^2(x_0)}{2m\beta\Delta}\sum_{l,n,j=1}^{\infty}\frac{[K^2(\theta_l)-K(\theta_l)K(\theta_n)]K(\theta_{j+n})}{A_l^2A_n^2A_j} \neq 0 , \tag{38}$$

$$\mu^2(x_0)=f'^2(x_0) +\frac{f''^2(x_0)}{m\beta\Delta}\sum_{l,n,j=1}^{\infty}\frac{[K(\theta_l)-K(\theta_n)]K(\theta_{j+l})}{A_l^2A_n^2A_j} . \tag{39}$$

Explicitly, the form of the trial frequency $\Omega^2(x_0)$ is different from that of conservative systems even for a harmonic potential system.

By construction, the variational result $W_1(x_0)$ for $W(x_0)$ becomes more accurate as the temperature is increased. In the low temperature case, because here two variational parameters are introduced, this variational approach is also expected to yield reliable results. This would be analyzed using Janke's method [6].

In summary, the theory presented in this paper accounts reliably for both quantum and dissipative effects. The two variational parameters corresponding to the frequency of the potential and the slope of the coupling form factor are determined by minimizing the effective potential with respect to $\Omega^2(x_0)$ and $\mu^2(x_0)$. It is also clear from studying a simple nonlinear dissipative example that the expression of the optimal affiliated frequency is different from that of conservative systems. In the future, more work needs to be done to apply this variational approach to a realistic open system with a large dissipative effect.

ACKNOWLEDGMENT

This work was supported by the National Natural Science Foundation of China.

[1] R. P. Feynman, *Statistical Mechanics* (Benjamin, Reading, MA, 1972).
[2] R. Giachetti and V. Tognetti, Phys. Rev. Lett. **55**, 912 (1985).
[3] R. P. Feynman and H. Kleinert, Phys. Rev. A **34**, 5080 (1986).
[4] H. Kleinert, Phys. Lett. A **118**, 267 (1986); W. Janke and H. Kleinert, *ibid.* **118**, 371 (1986).
[5] R. Giachetti and V. Tognetti, Phys. Rev. B **33**, 7647 (1986); A. R. McGurn, P. Ryan, A. A. Maradudin, and R. F. Wallis, *ibid.* **40**, 2407 (1989); A. Cuccoli and V. Tognetti, *ibid.* **41**, 9588 (1990); S. Liu, G. K. Horton, and E. R. Cowley, *ibid.* **44**, 11 714 (1991); A. Cuccoli, A. Macchi, V. Tognetti, and R. Vaia, *ibid.* **47**, 7859 (1993); **47**, 14 923 (1993).
[6] W. Janke, in *Path Integral from meV to MeV*, edited by V. Sa-Yakanit *et al.* (World Scientific, Singapore, 1989), pp. 355–365.
[7] R. Giachetti, V. Tognetti, A. Cuccoli, and R. Vaia, in *Ordering Phenomena in Condensed Matter,* edited by Z. Galasiewicz (World Scientific, Singapore, 1990), pp. 445–466.
[8] S. Liu, G. K. Horton, E. R. Cowley, A. R. McGurn, A. A. Maradudin, and R. P. Wallis, Phys. Rev. B **45**, 9716 (1992).
[9] H. Kleinert, Phys. Lett. A **173**, 332 (1993); J. Jaenicke and H. Kleinert, *ibid.* **176**, 409 (1993); H. Kleinert and H. Meyer, *ibid.* **184**, 319 (1994).
[10] U. Weiss, *Quantum Dissipative Systems* (World Scientific, Singapore, 1993), pp. 53–58.
[11] H. Grabert, P. Olschowski, and U. Weiss, Phys. Rev. B **36**, 1931 (1987).
[12] J.-D. Bao, Y.-Z. Zhuo, and X.-Z. Wu, Phys. Lett. B **327**, 1 (1994).